⑤ Radial Equation : $V(\vec{x}) = V(r)$

$$-\frac{\hbar^2}{2m}\left[\frac{\partial^2}{\partial r^2} + \frac{2}{r}\frac{\partial}{\partial r} + V_{\rm eff}^{(\ell)}(r)\right] R_{n\ell}(r) = E R_{n\ell}(r)$$

$\downarrow R \equiv \frac{u(r)}{r}$ $\qquad \| \quad V_{\rm eff}^{(\ell)}(r) = V(r) + \frac{\ell(\ell+1)}{2mr^2}\hbar^2$

… an effective potential.

$$-\frac{\hbar^2}{2m}\frac{d^2u}{dr^2} + V_{\rm eff}^{(\ell)}(r)\, u(r) = E\, u(r)$$

"

1D Schrödinger eq.

* normalization

$1 = \int r^2 dr |R|^2 = \int dr^2 |u|^2$

• Behavior at $r \to 0$.

We may write $u(r) \sim r^s$ at $r \to 0$ if it well-behaves.

$$\Rightarrow \underbrace{-\frac{\hbar^2}{2m} s(s-1) r^{s-2} + V(r) r^s + \frac{\ell(\ell+1)}{2m}\hbar^2 r^{s-2}}_{\text{Leading-order terms}} = E r^s$$

$\|$ assume that $r^2 V(r) \to 0$ as $r \to 0$.

$\Rightarrow s(s-1) = \ell(\ell+1)$

$\therefore s = \ell + 1$ or $\cancel{s = -\ell}$. unphysical!

why? Normalization

$\int_0^\infty dr\, r^{-2\ell}$: undefined when $\ell \geq 1$

if $\ell = 0$, $R \sim \frac{1}{r}$

$\to \nabla^2 \frac{1}{r} = 4\pi\delta(\vec{r})$.

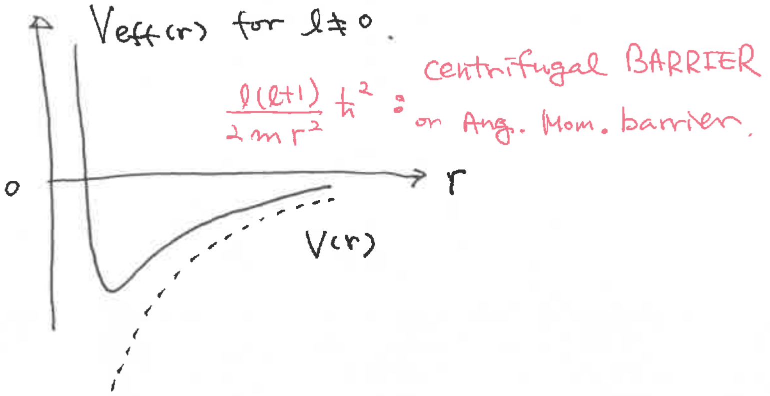
But the Schrödinger eq. has no source!

$\downarrow$

$$\boxed{R_{n\ell}(r) \sim r^\ell \text{ as } r \to 0.}$$

★ The wave fn. vanishes at $r=0$ unless $\ell = 0$.

$V_{\rm eff}(r)$ for $\ell \neq 0$.



⑥ Infinite Spherical Well : $V = \begin{cases} 0 & r<a \\ \infty & r>a. \end{cases}$

$$-\frac{\hbar^2}{2m}\left(\frac{d^2R}{dr^2} + \frac{2}{r}\frac{dR}{dr}\right) + \frac{l(l+1)}{2mr^2}\hbar^2 R = ER$$

by setting $k = \sqrt{\frac{2mE}{\hbar^2}}$, and $\rho = kr$

$$\rightarrow \frac{d^2R}{d\rho^2} + \frac{2}{\rho}\frac{dR}{d\rho} + \left[1 - \frac{l(l+1)}{\rho^2}\right]R = 0.$$

Sol. $R(\rho) = \begin{cases} j_l(\rho) = (-\rho)^l \left[\frac{1}{\rho}\frac{d}{d\rho}\right]^l \left(\frac{\sin\rho}{\rho}\right) & : \text{spherical Bessel fn.} \\ \cancel{n_l(\rho) = -(-\rho)^l \left[\frac{1}{\rho}\frac{d}{d\rho}\right]^l \left(\frac{\cos\rho}{\rho}\right)} & : \text{spherical Neumann fn.} \end{cases}$

But, $n_l(\rho) \rightarrow \rho^{-l-1}$ as $\rho \rightarrow 0$.

∴ unphysical!

$\therefore R(\rho) \propto j_l(\rho)$ → $\sim \rho^l$ as we argued it has to be.

boundary condition

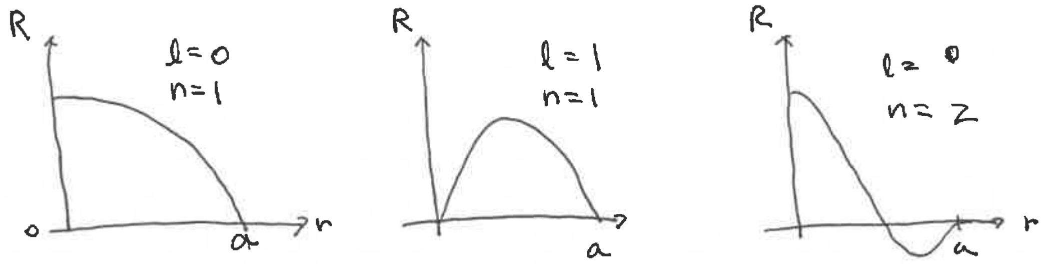
$j_l(ka) = 0$ → quantization of E.

ex. $l=0$: $j_0(ka) = \frac{\sin ka}{ka} = 0$

$\rightarrow ka = n\pi$

• $E_{l=0} = \frac{\hbar^2}{2m}\left(\frac{n\pi}{a}\right)^2$ // $n = 1, 2, 3, \cdots$

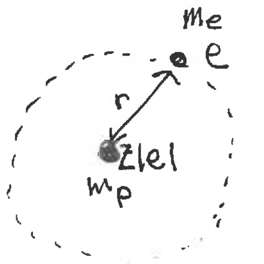
ex. $l=1$: $j_1(ka) = \frac{\sin ka}{(ka)^2} - \frac{\cos ka}{ka}$. : needs numerics to compute $E_{l=1}$.



⑦ The Hydrogen Atom

$$V(\vec{x}) = -\frac{Ze^2}{r}$$

"one-body problem"



Two-body problem.

r : relative coordinate.

$$m = \mu \quad : \text{reduced mass}$$

$$= \frac{m_e m_p}{m_e + m_p} \simeq m_e \quad (m_p \gg m_e)$$

$\Rightarrow$ radial equation : $$\left[-\frac{\hbar^2}{2m}\frac{d^2}{dr^2} + \frac{l(l+1)}{2mr^2}\hbar^2 - \frac{Ze^2}{r}\right]u = Eu$$

by setting $\rho \equiv kr$ where $k = \sqrt{\frac{2m|E|}{\hbar^2}}$ // $E<0$.

$$\Rightarrow \frac{d^2u}{d\rho^2} - \frac{l(l+1)}{\rho^2}u + \left(\frac{\rho_0}{\rho} - 1\right)u = 0$$

where $$\rho_0 = \sqrt{\frac{2m}{|E|}}\cdot\frac{Ze^2}{\hbar} = \sqrt{\frac{2mc^2}{|E|}}\cdot Z\alpha$$

($\alpha \equiv e^2/\hbar c \cong 1/137$: fine structure const.)

In the limit of $\rho \to \infty$,

$$\frac{d^2u}{d\rho^2} - u = 0 \quad \to \quad u \sim \begin{cases} e^{-\rho} \\ \cancel{e^{\rho}} \end{cases}$$ unphysical.

So, we can attempt to find a solution in the form of

$$u(\rho) = \rho^{l+1} e^{-\rho} w(\rho).$$

$$\Rightarrow \rho\frac{d^2w}{d\rho^2} + 2(l+1-\rho)\frac{dw}{d\rho} + [\rho_0 - 2(l+1)]w(\rho) = 0$$

Try a power-series solution

$$w(\rho) = \sum_{k=0}^{\infty} c_k \rho^k \qquad // \; c_0 \neq 0 \,!$$

to keep the behavior at $r \to 0$.

$$\Rightarrow \sum_{k=2}^{\infty} C_k \cdot k \cdot (k-1)\rho^{k-1} + 2(\ell+1)\sum_{k=1}^{\infty} C_k \cdot k \cdot \rho^{k-1}$$

$$-2\sum_{k=1}^{\infty} C_k \cdot k \cdot \rho^k + [\rho_0 - 2(\ell+1)]\sum_{k=0}^{\infty} C_k \rho^k = 0$$

$$\Rightarrow \sum_{k=\cancel{1}\to 0}^{\infty} C_{k+1}(k+1)\cdot k\,\rho^k + \sum_{k=0}^{\infty}(2\ell+2)C_{k+1}(k+1)\rho^k$$

$$+\sum_{k=\cancel{1}\to 0}^{\infty}(-2)C_k \cdot k \cdot \rho^k + [\rho_0 - 2(\ell+1)]\sum_{k=0}^{\infty} C_k \rho^k = 0$$

$$\Rightarrow \sum_{k=0}^{\infty}\Big[[k(k+1)+2(\ell+1)(k+1)]C_{k+1} - [2k+2(\ell+1)-\rho_0]C_k\Big]\rho^k = 0$$

$$\therefore \frac{C_{k+1}}{C_k} = \frac{2k+2\ell+2-\rho_0}{(k+1)(k+2\ell+2)} \sim \frac{2}{k} \text{ as } k\to\infty.$$

[if ρ_0 is not an positive integer.]

: This is a problem,

because $\frac{C_{k+1}}{C_k} \sim O\left(\frac{1}{k}\right)$ gives $w(\rho) \sim \exp[2\rho]$,

and then it changes the asymptotic behavior.

$\Rightarrow$ Therefore, the term C_k has to be terminated at some power $k=N$, s.t.

$$\therefore \rho_0 = \boxed{\text{positive integer}} = 2(N+\ell+1) \equiv 2n$$

$$\Rightarrow E = -\underbrace{\frac{1}{2}mc^2(Z\alpha)^2}_{13.6\,\text{eV}\cdot Z^2}\frac{1}{n^2} \quad \Big\| \quad n = \underline{N+\ell+1} = 1, 2, 3, 4 \cdots$$

(N: 0, 1, 2, ⋯; ℓ: 0, 1, 2, ⋯)

"principal quantum number"

$\Rightarrow$ $n=1$ ⋯ $\ell=0$ only allowed.

$n=2$ ⋯ $\ell=0, 1$

$n=3$ ⋯ $\ell=0, 1, 2$.

⋮

degeneracy of E_n $\leftarrow$ # of $|n,l,m\rangle$ for a given n.

$$= \sum_{l=0}^{n-1} 2l+1 = n^2$$

- The length scale κ in $\rho = \kappa r$ also n-dependent!

$$\frac{1}{\kappa} = \frac{\hbar}{mc\alpha}\frac{n}{Z} \equiv a_0 \frac{n}{Z}$$

$\rightarrow$ natural length scale $a_0 \equiv \frac{\hbar^2}{mc\alpha} = \frac{\hbar^2}{me^2}$: Bohr radius

- finally, the wave ~~function~~ :

$$\psi_{nlm}(\vec{x}) = R_{nl}(r)\, Y_l^m(\theta,\phi).$$

$$R_{nl}(r) = \left(\frac{Z}{na_0}\right)^l \cdot e^{-\frac{Zr}{na_0}} \sum_{k=0}^{\infty} C_k \left(\frac{Z}{na_0} r\right)^k$$

where $$\frac{C_{k+1}}{C_k} = \frac{2(k+l+1-n)}{(k+1)(k+2l+2)}.$$

, C_0 has to be determined by the normalization

$$\int_0^\infty r^2 dr\, |R_{nl}|^2 = 1.$$

- The other example in the S&N is the isotropic simple Harmonic Oscillator.

$\leftarrow$ Try to solve it by yourself.

Caution: the asymptotic behavior at a large r is different.

* Implications of the degeneracy "n^2": Is it accidental?

(S&N. ch.4.1)

for a given n, $l = 0, 1, \cdots n-1$ are allowed.

→ Maybe there exists some symmetry higher than $SO(3)$.

[$SO(3)$ indicates only $m = -l \cdots l$ for a given l.]

- In the Kepler problem in C.M. ($F(\vec{r}) = -\frac{k}{r^2}\hat{r}$)

$$\vec{A} = \vec{p} \times \vec{L} - mk\hat{r} \quad \text{is conserved.}$$

: Laplace – Runge – Lenz or Runge-Lenz or Lenz vector.

→ The perihelion does not change in time.

- In Q.M., a Hermitian version of the Lenz vector:

$$\vec{M} = \frac{1}{2m}(\vec{p} \times \vec{L} - \vec{L} \times \vec{p}) - \frac{Ze^2}{r}\vec{x}$$

For two Hermitian $\vec{A}, \vec{B}$, $(\vec{A} \times \vec{B})^\dagger = -\vec{B} \times \vec{A}$

$$\Rightarrow [\vec{M}, H] = 0 \quad !!! \quad \text{for } H = \frac{\vec{p}^2}{2m} - \frac{Ze^2}{r}$$

one can also find

$$\vec{L} \cdot \vec{M} = \vec{M} \cdot \vec{L} = 0$$

$$\vec{M}^2 = \frac{2}{m} H (\vec{L}^2 + \hbar^2) + Z^2 e^4,$$

and

$$[L_i, L_j] = i\hbar \varepsilon_{ijk} L_k$$
$$[M_i, M_j] = -i\hbar \varepsilon_{ijk} \frac{2}{m} H L_k$$
$$[M_i, L_j] = i\hbar \varepsilon_{ijk} M_k$$

This prevents us to make a closed algebra, but, we can make it closed by considering energy eigenstates → $H = E$.

$$\Downarrow$$

$$[L_i, L_j] = i\hbar \varepsilon_{ijk} L_k$$
$$[N_i, N_j] = i\hbar \varepsilon_{ijk} L_k$$
$$[N_i, L_j] = i\hbar \varepsilon_{ijk} N_k.$$

$$\Leftarrow \quad \vec{N} \equiv \left(-\frac{m}{2E}\right)^{\frac{1}{2}} \vec{M}$$

★ 6 generators of $SO(4)$. : rotations in 4D.

But, we can seperate the algebra of $SO(4)$ into two sets of algebras.

NOTE: $[\vec{I}, H] = 0$, $[\vec{K}, H] = 0$

If we define
$$\left[\begin{array}{l} \vec{I} \equiv (\vec{L} + \vec{N})/2 \\ \vec{K} \equiv (\vec{L} - \vec{N})/2 , \end{array}\right.$$

★

$$\Rightarrow [I_i, I_j] = i\hbar \varepsilon_{ijk} I_k , \quad [K_i, K_j] = i\hbar \varepsilon_{ijk} K_k , \quad [I_i, K_j] = 0$$

$\downarrow SU(2)$ $\qquad\qquad\qquad \downarrow SU(2)$

$I^2 \to i(i+1)\hbar^2$ $\quad \| \, i = 0, \frac{1}{2}, 1, \frac{3}{2}, \cdots$
$(2i+1)$ deg.

$K^2 \to k(k+1)\hbar^2$ $\quad \| \, k = 0, \frac{1}{2}, 1, \frac{3}{2}, \cdots$
$(2k+1)$ deg.

Since $\vec{I}^2 - \vec{K}^2 = \vec{L} \cdot \vec{N} = 0$, $k = i$.

The operator $\vec{I}^2 + \vec{K}^2 = \frac{1}{2}\left[\vec{L}^2 - \frac{m}{2E}\vec{M}^2\right]$

goes to $2k(k+1)\hbar^2 = \frac{1}{2}\left(-\hbar^2 - \frac{m}{2E} Z^2 e^4\right)$ //

$\| \; \vec{M}^2 = \frac{2}{m} H(\vec{L}^2 + \hbar^2) + Z^2 e^4$.

$\downarrow$

$$E = -\frac{mZ^2e^4}{2\hbar^2}\frac{1}{(2k+1)^2}, \quad k = 0, \frac{1}{2}, 1, \frac{3}{2}, \cdots \; ☆$$

$$= -\frac{mZ^2e^4}{2\hbar^2}\frac{1}{n^2}, \quad n = 1, 2, 3, 4, \cdots$$

$\therefore$ deg. $= (2i+1)\cdot(2k+1)\Big|_{k=i}$ for a given n.

$= n^2$

$SO(4) = SU(2) \times SU(2)$